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ADAPTIVE CURVE FITTING FOR CHEMICAL PROCESSES. (U)

JUL 77 M ANDREWS, J A HULL, G D TAYLOR

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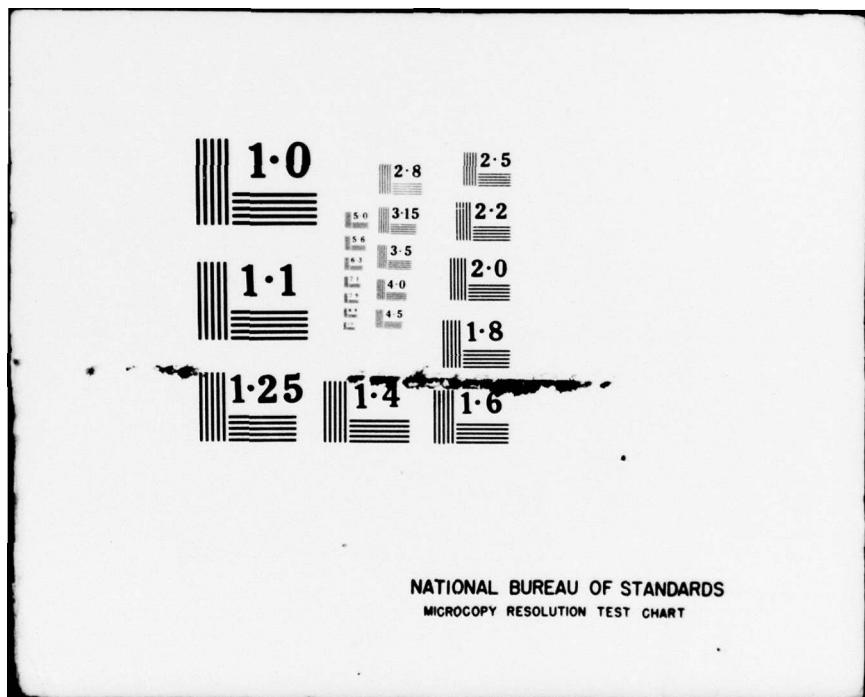
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Adaptive Curve Fitting for Chemical Processes

M. Andrews¹, J. A. Hull² and G. D. Taylor²

I. Introduction

Closed-loop control systems for many chemical processes require accurate modeling of the system. Typically, such models are generated by assuming that a set of differential equations can be found which describe system dynamics. (In chemical processes, a kinetic analysis is applied to chemical species reactions (system dynamics) which may be linear (first-order) or non-linear (second-order) [1,2].) The differential equations are then imbedded in the modeling behavior of the closed-loop control system.

Generally, a least squares fit is performed on empirical data to identify reaction models with a set of differential equations which are then used in the control phase [3]. During on-line control operations, these differential equations are solved by iterative numerical methods such as (Runge-Kutta, Adams-Moulton) to identify point-wise values upon which the model values are compared to the on-line data. The result of this comparison is an error or feedback signal which drives the control system of the chemical process. An inherent drawback of this technique is that employment of differential equations requires recursive numerical calculations which may amplify modeling errors as time proceeds, eventually causing the system to diverge. It thus appears desirable to minimize or at least identify modeling uncertainties a priori.

¹M. Andrews is with the Dept. of Electrical Engineering, J. Hull and G. Taylor are with the Mathematics Dept.. Colorado State University, Fort Collins, Colorado.

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An alternative procedure, described herein, is to curve fit the data with a (smooth) piecewise polynomial with known error bounds. Since the modeling errors for curve fitting techniques of this paper can be determined beforehand, a prescribed tolerance band or error bound can be identified at the onset, and (in general) piecewise polynomial approximations can be found satisfying this tolerance. This procedure uses algorithms described in [4,5] for curve fitting which splice Nth degree polynomials together meeting user defined smoothness and error tolerances. The points at which this splicing occurs are called knots. The knots (where and how many) and the individual polynomials are the free parameters. This technique differs from previous methods in that the error tolerances are specified first and the knots are automatically placed. The application of this algorithm in an interactive mode which could make use of an operator controlled CRT strategy for initially specifying knot locations and terminally overriding the algorithm's automatic features, if past experience with the particular data indicates otherwise.

II. Algorithm

Our algorithms compute smooth piecewise polynomial approximations within a user selected tolerance to a given data set using best (discrete) L^2 approximations or best restricted range uniform approximations; the number and location of the "knots" or "joints" of the polynomial pieces are automatically determined by the algorithms. More specifically, suppose we wish an approximation

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to the data

$$\{(t_v, y_v)\}_{v=0}^m, \text{ where } t_{v-1} < t_v, v = 1, 2, \dots, m.$$

Our algorithms will distinguish $\ell + 1$ of the t_v 's, say $t_0 = x_0$, $x_1, x_2, \dots, x_\ell = t_m$ ($x_{v-1} < x_v, v = 1, 2, \dots, \ell$) as knots and associated with these knots the algorithms will find (or at least attempt to find) polynomials, p_1, p_2, \dots, p_ℓ with the following properties:

- i) Each p_i has degree less than or equal to $N-1$, where N is a user defined positive integer. (N represents the allowable number of coefficients for any p_i);
- ii) $p_i^{(j)}(x_i) = p_{i+1}^{(j)}(x_i)$ for $i = 1, 2, \dots, \ell - 1$, and for $j = 0, 1, \dots, \text{SMTH}$, where SMTH is a user defined integer ($\text{SMTH} \leq N$) which represents the number of continuous derivatives required of the piecewise polynomial approximation.
- iii) a) If we are using the L^2 algorithm, and if $x_{i-1} \leq t_j \leq x_i$, then we have that $|p_i(t_j) - y_j| \leq \text{TOL}$, where TOL is a positive quantity representing the tolerance the user requires the approximation to satisfy. Moreover, p_i is the best (discrete) L^2 approximation to the data $\{(t_v, y_v) : s_{i-1} \leq t_v \leq x_i\}$ of degree less than or equal to $N - 1$, subject to the interpolatory constraints imposed by ii) above.
- iii) b) If we are using the restricted range algorithm, the user supplies numbers $\{L_v\}_{v=0}^m$ and $\{U_v\}_{v=0}^m$ such that $L_v \leq y_v \leq U_v$, $v = 0, 1, \dots, m$ (which, in effect, define an allowable tolerance at each data point. We shall refer to these numbers as restraining curves) and the polynomials, p_i , have the property that whenever

t_j is such that $x_{i-1} \leq t_j \leq x_i$ for some fixed i , $L_j \leq p_i(t_j) \leq U_j$. Moreover, p_i is the best restricted range uniform polynomial approximation to $\{(t_v, y_v) : x_{i-1} \leq t_v \leq x_i\}$ of degree less than or equal to $N - 1$ subject to the interpolatory constraints imposed by ii) above.

For complete descriptions and FORTRAN listings of these algorithms see [4], and [5].

III. Numerical examples and suggestions for effective use

As an example, in this paper, we have applied our technique to the problem of the mathematical modeling of the kinetics of oil shale pyrolysis [6]. The Hubbard and Robinson data set [6] was utilized to fit piecewise polynomials of degree 5 with two continuous derivatives to the oil and gas yield data and bitumen yield data at 475° and 425° isotherms.

Because there are only 15-20 points in each data set, which is too few for effective use of these algorithms, we linearly interpolated the data and then discretized these curves so that we approximated on a set of 200 to 500 data points in each of these examples. Since our algorithms do not require the data points to be equally spaced, we packed points more densely where the data is complicated, and more sparsely where the data is smooth. Although it is computationally more expensive, in general, better approximations result if one approximates on more (densely packed) data points. In fact, often if an algorithm returns an approximation with oscillatory problems, or if an algorithm cannot meet a specified tolerance, these problems can be overcome by adding more (densely packed) data points by means of this simple linear interpolation scheme.

We now give several examples. In all of the following graphs, the data points being approximated are indicated by "x", and the small boxes indicate the location of the knots. When using the restricted range algorithm, the restraining curves have been hand fitted or fitted using a simple algorithm which sets the restraining curves according to the complexity of the function.

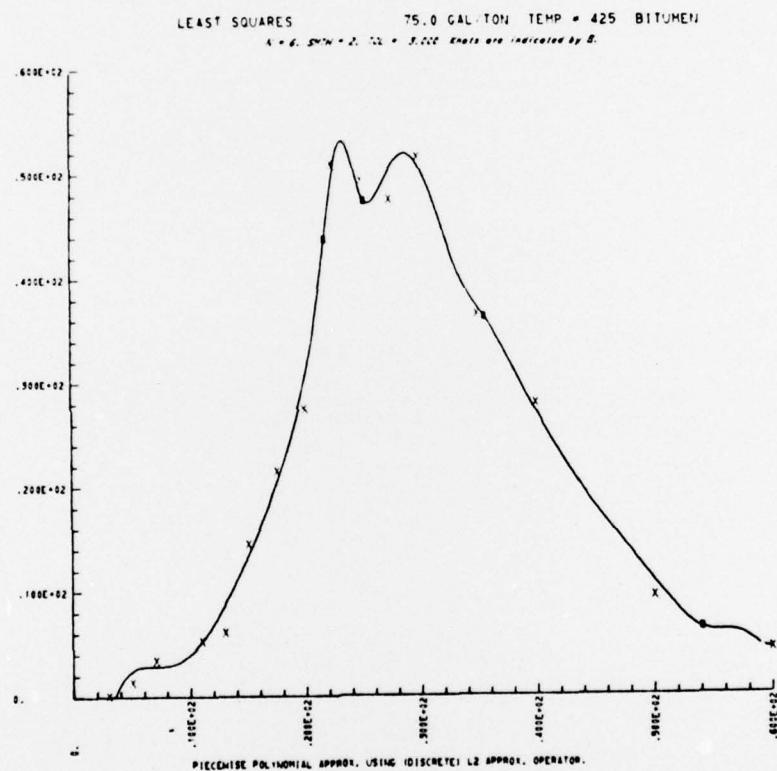


Figure 1

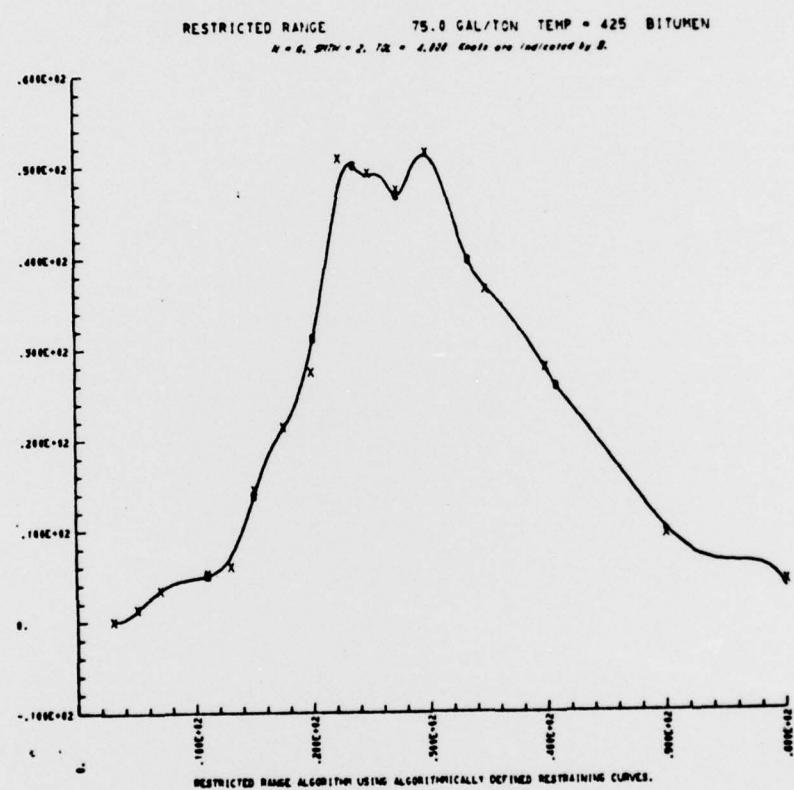


Figure 2

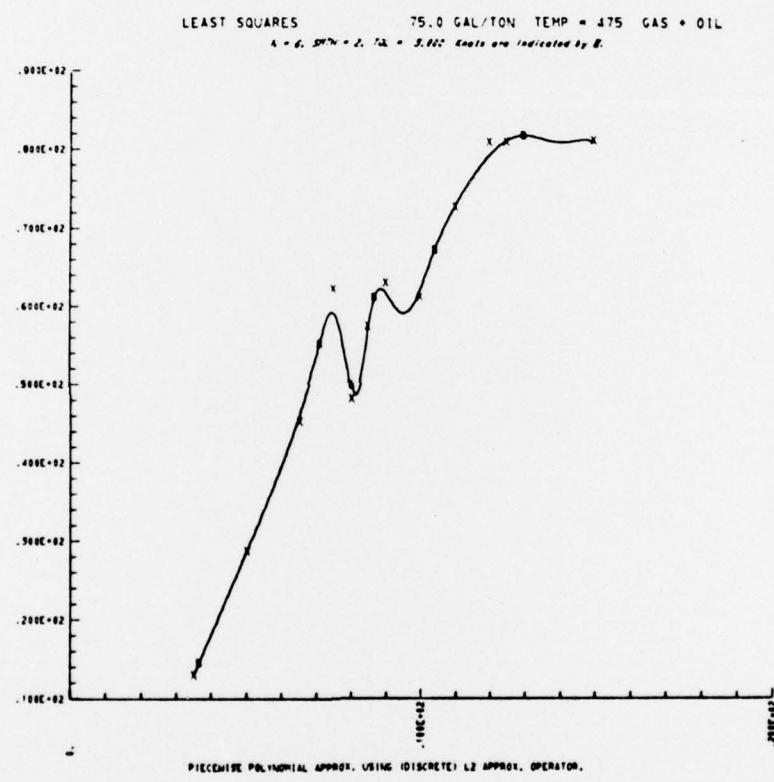


Figure 3

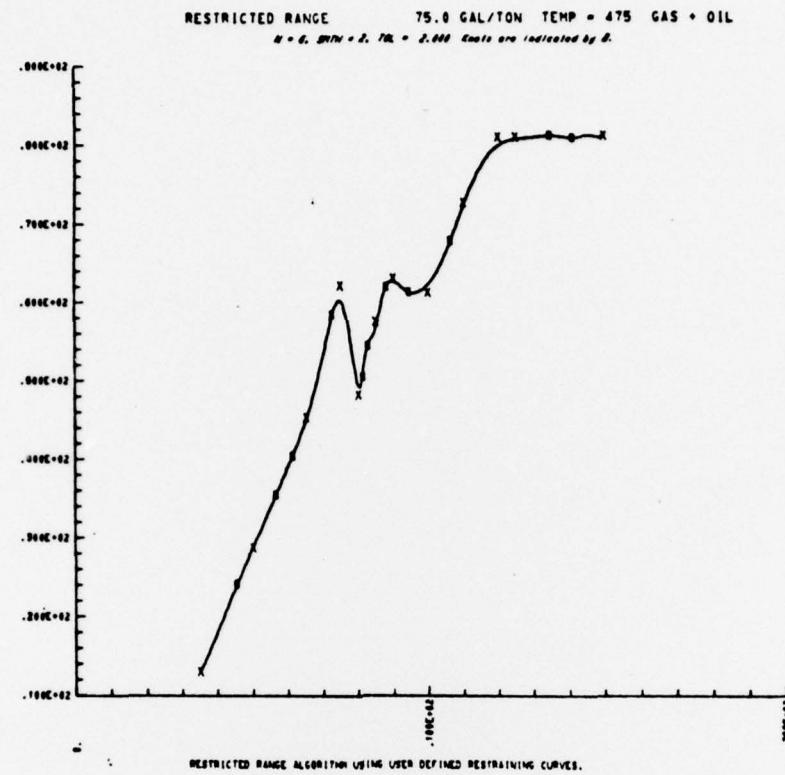


Figure 4

Note that in the above examples we were able to force the shape of the approximation to more closely follow the shape of the functions being approximated but at a cost of more knots. By setting tolerance bands containing the data as in the following example, we take advantage of the restricted range algorithm's capability of forcing the approximation to lie within certain bounds while still allowing the approximation a much higher degree of freedom than in the above examples. We also illustrate our choice of restraining curves.

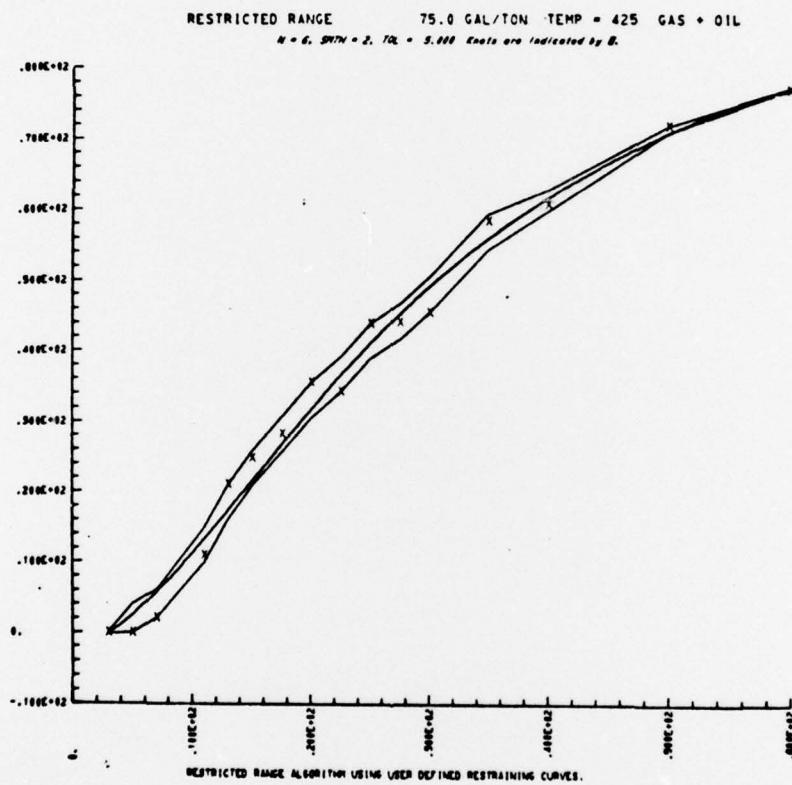


Figure 5

For clarity we repeat this example without the restraining curves.

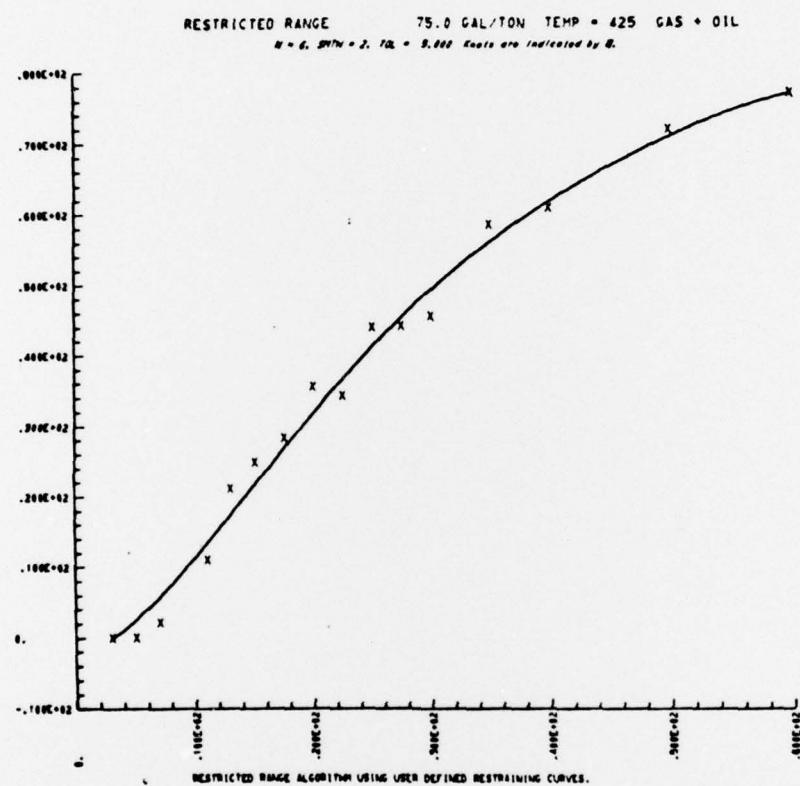


Figure 6

Next we show the same example with much tighter tolerances.

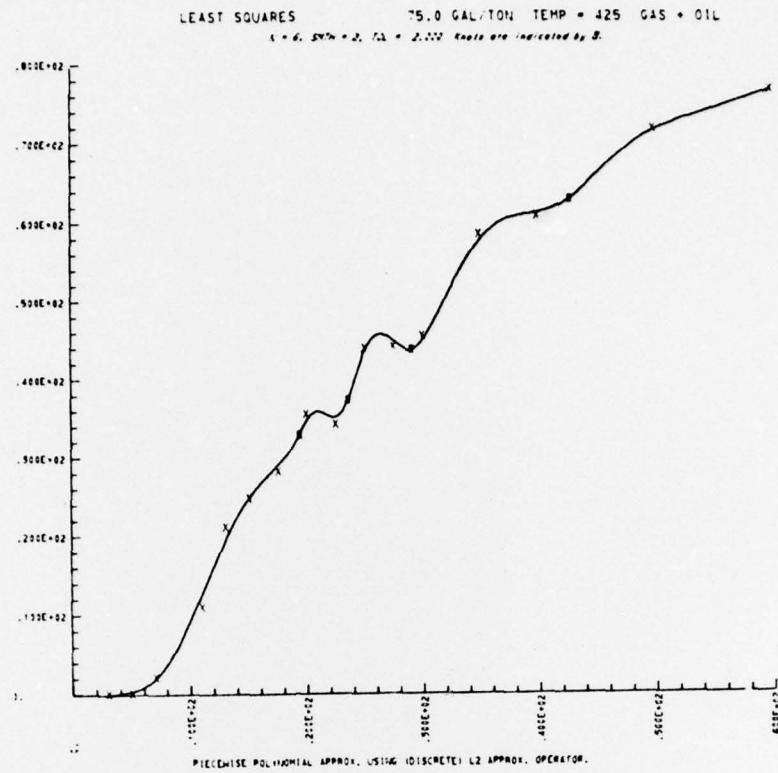


Figure 7

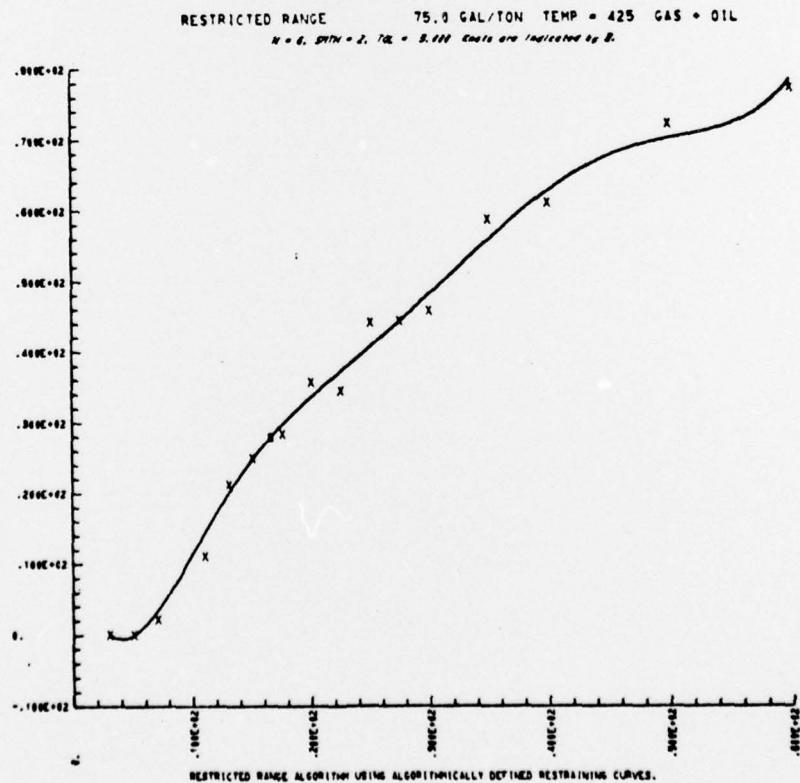


Figure 8

As noted above, we required approximations determined by the restricted range algorithm to agree very closely to the function being approximated where the function was "nice". The following example illustrates that setting the tolerances too small in these areas can be costly in terms of numbers of knots. By setting the tolerances as small as we did throughout the "smooth" regions of the function, we essentially required our approximation to be nearly linear since we were approximating linearly interpolated data.

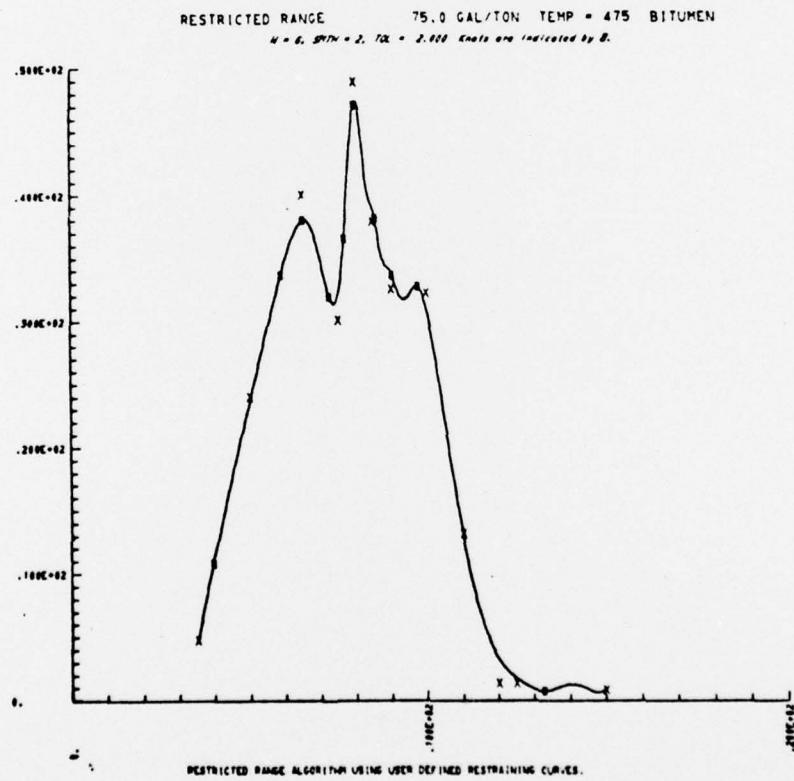


Figure 9

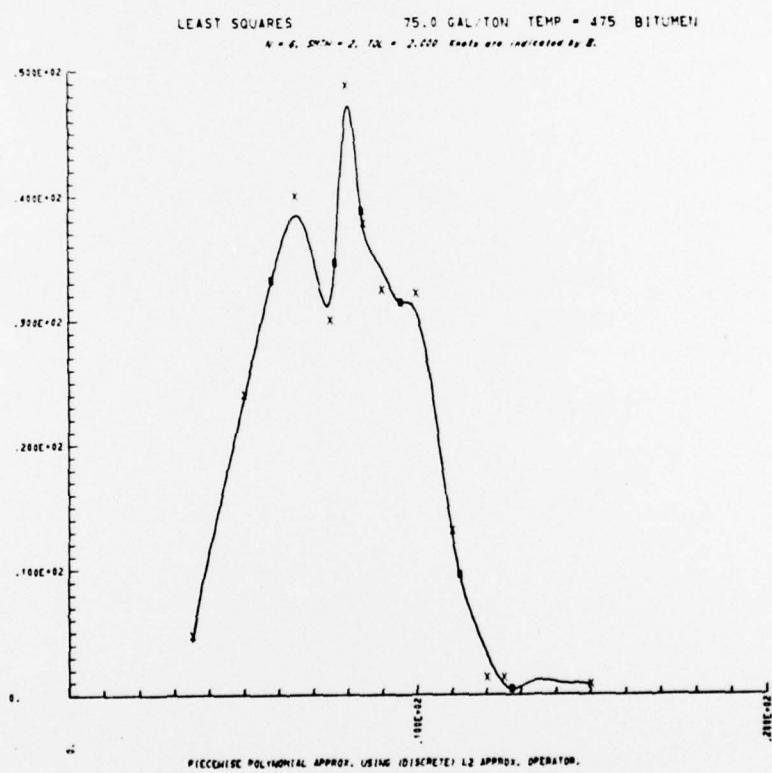


Figure 10

The restricted range algorithm, though more complicated than the L^2 algorithm, allows the user much more flexibility in setting tolerances the approximation must satisfy. By appropriately setting the numbers $\{U_v\}$ and $\{L_v\}$, the user can vary the tolerance requirement throughout the domain of the approximation and, to a large extent, determine the shape of the resulting approximation. Ideally, these restraining curves would be determined in an interactive setting using a graphics terminal with a pen-light, as follows. First, one would make a rough initial guess at what the restraining curves should be (by some simple algorithm or otherwise), then allow the algorithm to compute the first piece of the approximation. One would next display the data, the current approximation and the current restraining curves and then modify the restraining curves on the relevant subinterval as desired so that when this first piece is recomputed using the updated restraining curves, it behaves as desired. After the user is satisfied with the first piece, he would repeat the above strategy on each successive subinterval determined by the algorithm.

As is the case with any smooth piecewise polynomial approximation algorithm, "good" placement of the knots is critical for "good" approximations. While our algorithms attempt to find "good" locations for the knots, sometimes the user may be able to find by inspection locations which would be more optimal. Again, if the interactive mode and a graphics terminal is available to the user, the straight-forward left to right joining strategy of our algorithms facilitate the implementation of a scheme

whereby the user could choose the location of the next knot (or the general vicinity of the knot and have the algorithm optimize the location in that vicinity), overriding the algorithms' automatic choice, when he can identify a "better" knot location.

We recommend these curve fitting algorithms when one wishes to approximate data with an a priori error estimate. If the user needs an approximation to reflect certain features of the approximant, or when approximating data in which there are varying levels of noise, the restricted range algorithm should be used. When a more automatic and simple to use algorithm is desired, the L^2 algorithm should be used.

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